

Calculation of parity non-conservation in xenon and mercury

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We use configuration interaction technique to calculate parity non-conservation (PNC) in metastable Xe and Hg [proposal of the experiment in L. Bougas *et al*, Phys. Rev. Lett. **108**, 210801 (2012)]. Both, nuclear spin-independent and nuclear spin-dependent (dominated by the nuclear anapole moment) parts of the amplitude are considered. The amplitudes are strongly enhanced by proximity of the states of opposite parity.

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I. INTRODUCTION

The study of the parity non-conservation in atoms is a low-energy, relatively inexpensive alternative to high-energy search for new physics beyond the standard model (see, e.g. [1–3]). For example, parity non-conservation in cesium is currently the best low-energy test of the electroweak theory [1, 3]. It is due to high accuracy of the measurements [4] and its interpretation [5] (see also [6]). Since the cesium result is unlikely to be significantly improved, the focus of the PNC study in atoms has shifted to two important areas: (i) the PNC measurements for a chain of isotopes and (ii) the measurements of nuclear anapole moment (see, e.g. [3]). Most of current or planned PNC experiments in atoms consider both possibilities.

The experiments are in progress at Berkeley for Dy and Yb atoms [7, 8], at TRIUMF for Rb and Fr atoms [9, 10], and at Groningen (KVI) for Ra^+ ions [11]. There is an interesting recent suggestion to measure PNC in metastable Xe and Hg [12]. In the present paper we support this proposal by the atomic calculations.

The advantages of using Xe and Hg for the measurements of PNC in a chain of isotopes and the measurements of anapole moments include: (i) large number of stable isotopes of both atoms (maximal difference in the number of neutrons is $\Delta N = 12$ for Xe and $\Delta N = 8$ for Hg); (ii) presence of two stable isotopes for each of the atoms with non-zero nuclear spin (^{129}Xe , $I = 1/2$; ^{131}Xe , $I = 3/2$; ^{199}Hg , $I = 1/2$; ^{201}Hg , $I = 3/2$), these isotopes are suitable for the anapole moment measurements; (iii) The PNC amplitudes in the Xe and Hg atoms are enhanced due to the high nuclear charge and strong mixing with close states of opposite parity.

An extra advantage comes from the fact that xenon and mercury nuclei with non-zero spin have valence neutron, therefore the nuclear anapole measurements will provide the strength constant for the neutron-nucleus PNC potential. The anapole moment so far was measured only for ^{133}Cs [4] which has valence proton. The data for the xenon and mercury would be complementary to those obtained for cesium.

In the present work we use the configuration interaction (CI) technique to calculate the nuclear spin-

independent PNC amplitudes caused by the weak nuclear charge and the nuclear spin-dependent PNC amplitudes dominated by the nuclear anapole moments. The result is presented in a convenient form as a sum of two contributions for different hyperfine structure components. This would allow to extract both the value and the sign of the anapole moments by comparing the measured amplitudes with the calculated ones.

II. GENERAL FORMALISM

The Hamiltonian describing parity-nonconserving electron-nuclear interaction can be written as a sum of the nuclear-spin-independent (SI) and the nuclear-spin-dependent (SD) parts (we use atomic units: $\hbar = |e| = m_e = 1$):

$$\begin{aligned} H_{\text{PNC}} &= H_{\text{SI}} + H_{\text{SD}} \\ &= \frac{G_F}{\sqrt{2}} \left(-\frac{Q_W}{2} \gamma_5 + \frac{\kappa}{I} \boldsymbol{\alpha} \mathbf{I} \right) \rho(\mathbf{r}), \end{aligned} \quad (1)$$

where $G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, Q_W is the nuclear weak charge, $\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$ and γ_5 are the Dirac matrices, \mathbf{I} is the nuclear spin, and $\rho(\mathbf{r})$ is the nuclear density normalized to 1. The strength of the spin-dependent PNC interaction is proportional to the dimensionless constant κ which is to be found from the measurements. There are three major contributions to κ arising from (i) electromagnetic interaction of atomic electrons with the nuclear *anapole moment* [13], (ii) electron-nucleus spin-dependent weak interaction [14], and (iii) combined effect of spin-independent weak interaction and magnetic hyperfine interaction [15] (see also [1]). In this work we do not distinguish between different contributions to κ and present the results in terms of total κ which is the sum of all possible contributions.

Within the standard model the weak nuclear charge Q_W is given by [16]

$$Q_W \approx -0.9877N + 0.0716Z. \quad (2)$$

Here N is the number of neutrons, Z is the number of protons.

The PNC amplitude of an electric dipole transition between states of the same parity $|i\rangle$ and $|f\rangle$ is equal to:

$$E1_{fi}^{PNC} = \sum_n \left[\frac{\langle f|\mathbf{d}|n\rangle\langle n|H_{PNC}|i\rangle}{E_i - E_n} + \frac{\langle f|H_{PNC}|n\rangle\langle n|\mathbf{d}_q|i\rangle}{E_f - E_n} \right], \quad (3)$$

where $\mathbf{d} = -e \sum_i \mathbf{r}_i$ is the electric dipole operator. To extract from the measurements the parameter of the nuclear spin-dependent weak interaction \varkappa one needs to consider PNC amplitudes between specific hyperfine structure components of the initial and final states. There amplitudes can be expressed as

$$E1_{fi}^{PNC} = (-1)^{F_f - M_f} \begin{pmatrix} F_f & 1 & F_i \\ -M_f & q & M_i \end{pmatrix} \times \langle J_f F_f || d_{PNC} || J_i F_i \rangle. \quad (4)$$

Here $\mathbf{F} = \mathbf{J} + \mathbf{I}$, \mathbf{I} is nuclear spin. Detailed expressions for the reduced matrix elements of the SI and SD PNC amplitudes can be found e.g. in Refs. [17] and [18]. For the SI amplitude we have

$$\begin{aligned} \langle J_f, F_f || d_{SI} || J_i, F_i \rangle &= (-1)^{I + F_i + J_f + 1} \\ &\times \sqrt{(2F_f + 1)(2F_i + 1)} \begin{Bmatrix} J_i & J_f & 1 \\ F_f & F_i & I \end{Bmatrix} \\ &\times \sum_n \left[\frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n || H_{SI} || J_i \rangle}{E_i - E_n} + \frac{\langle J_f || H_{SI} || n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_f - E_n} \right] \\ &\equiv c(F_f, J_f, F_i, J_i) E'_{fi}. \end{aligned} \quad (5)$$

Here $c(F_f, J_f, F_i, J_i)$ is the angular coefficient and the sum over n , E'_{fi} does not depend on F_f or F_i :

$$E' = \sum_n \left[\frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n || H_{SI} || J_i \rangle}{E_i - E_n} + \frac{\langle J_f || H_{SI} || n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_f - E_n} \right]. \quad (6)$$

For the SD PNC amplitude we have

$$\begin{aligned} \langle J_f, F_f || d_{SD} || J_i, F_i \rangle &= \frac{G_F}{\sqrt{2}} \varkappa \\ &\times \sqrt{(I + 1)(2I + 1)(2F_i + 1)(2F_f + 1)/I} \\ &\times \sum_n \left[(-1)^{J_f - J_i} \begin{Bmatrix} J_n & J_i & 1 \\ I & I & F_i \end{Bmatrix} \begin{Bmatrix} J_n & J_f & 1 \\ F_f & F_i & I \end{Bmatrix} \right. \\ &\times \frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n || \alpha \rho || J_i \rangle}{E_n - E_i} \\ &+ (-1)^{F_f - F_i} \begin{Bmatrix} J_n & J_f & 1 \\ I & I & F_f \end{Bmatrix} \begin{Bmatrix} J_n & J_i & 1 \\ F_i & F_f & I \end{Bmatrix} \\ &\times \left. \frac{\langle J_f || \alpha \rho || n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_n - E_f} \right]. \end{aligned} \quad (7)$$

TABLE I: Energy levels (in cm^{-1}) and g -factors of low states of mercury. States considered for the PNC transitions are marked as A and B.

Configu- ration	State	Calculations		Experiment	
		Energy	g	Energy	g
$6s^2$	1S_0	0	0.000	0	0.000
$6s6p$	A ₁	$^3P_0^o$	38202	0.000	37645
	A ₂	$^3P_1^o$	39955	1.480	39412
	A ₃	$^3P_2^o$	44812	1.500	44043
	B	$^1P_1^o$	53584	1.020	54069
$6s7s$	3S_1	61879	2.000	62350	2.003
	1S_0	63399	0.000	63928	0.000

TABLE II: Energy levels (in cm^{-1}) and g -factors of low states of xenon. States considered for the PNC transition are marked as A and B.

Configu- ration	J	Calculations		Experiment	
		Energy	g	Energy	g
$5p^6$	0	0	0.000	0	0.000
$5p^56s$	A	2	64680	1.500	67068
		1	66089	1.214	68046
		0	74844	0.000	76197
$5p^56p$	B	1	75999	1.314	77186
		1	76083	1.853	77270
		1	77914	1.024	78957

The PNC amplitude between different hfs components of the initial and final states can be presented in a form

$$E_{PNC}(F_1, F_2) = c(F_1, F_2) E' Q_w [1 + R(F_1, F_2) \varkappa], \quad (8)$$

where c is an angular coefficient and R is the ratio of the spin-dependent to the spin-independent PNC amplitudes.

If at least two PNC amplitudes E_1 and E_2 are measured then the value of \varkappa can be expressed via the measured ratio of the amplitudes E_1/E_2 and the calculated ratios R of the SD and SI PNC amplitudes.

$$\begin{aligned} E_1 &= c_1 E' Q_W (1 + R_1 \varkappa), \\ E_2 &= c_2 E' Q_W (1 + R_2 \varkappa), \end{aligned} \quad (9)$$

$$\varkappa = \frac{c_1/c_2 - E_1/E_2}{R_2 E_1/E_2 - R_1 c_1/c_2}. \quad (10)$$

The ratios R_1, R_2 are much less sensitive to numerical uncertainties than each of the SD and SI PNC amplitudes [19].

III. CALCULATIONS

Calculations for xenon and mercury were performed with the use of the configuration interaction (CI) method. We treat Hg as an atom with two valence electrons and Xe as an atom with six valence electrons. Calculations for Hg are very similar to what we did before for Hg [20]

and Yb [21]. We use the V^{N-2} approximation in which initial Hartree-Fock procedure is done for the Hg^{2+} ion. The complete set of single-electron orbitals is constructed using the B-spline technique [22]. Core-valence correlations are included by adding the second-order correlation potential $\hat{\Sigma}$ to the CI Hamiltonian in the framework of the CI+MBPT method [23]. Accuracy for the energies is further improved by rescaling the core-valence correlation operator Σ (see [20, 21] for details). The rescaling coefficients are $\lambda_s = 0.82$ for s -states and $\lambda_p = 0.9$ for p -states. The calculated energies and g -factors of mercury are presented in Table I together with corresponding experimental numbers. The g -factors are useful for the identification of states. The accuracy for the calculated energies is within 1% for majority of the states. It is not perfect in spite of the fitting because with use only two fitting parameters for all states.

Similar approach for xenon is problematic due to the larger number of valence electrons. We treat all $5p$ electrons as valence ones, so that total number of valence electrons is six. Using the same technique as for Hg would lead to a very large CI matrix. It was suggested in [12] that the hole-particle formalism can be used for the calculation of the electron structure of xenon. In this case only two active particles enter the CI calculations and the calculations might not be more complicated than for mercury. This assumes that only single excitations are allowed from the $5p$ subshell. However, in our experience double excitations are also important. Inclusion of double excitations within the hole-particle formalism hugely complicates the problem. Therefore, we use simpler approach. We use standard CI technique for six valence electrons. Initial Hartree-Fock procedure is done for neutral xenon (the V^N approximation). Single-electron basis states above the core are calculated as the Hartree-Fock states in the V^{N-1} potential of the frozen core. Many-electron basis states for the CI calculations are formed by allowing single and double excitations from the $5p$ subshell to the states above the core.

Accurate treatment of the core-valence correlations for xenon within the CI+MBPT method is problematic due to large contribution of the subtraction diagrams [23]. On the other hand the core-valence correlations are relatively small for xenon compared to valence-valence correlations due to large number of valence electrons. Therefore, they can be included approximately.

To simulate the effect of core-valence correlations we include into the CI Hamiltonian the core polarization potential

$$\delta V = -\frac{\alpha_c}{a^4 + r^4}, \quad (11)$$

where α_c is the polarizability of the core and a is a cut-off parameter. We use $a = a_B$ and treat α_c as a fitting parameter. This allows us to fit the energy interval $\Delta E = 84 \text{ cm}^{-1}$ between state B and close state of the same total momentum J and opposite parity belonging to the $5p^5 6p$ configuration. This is important because PNC amplitude is very sensitive to this energy interval. We use $\alpha_c =$

0.554 a.u. for s states of valence electrons and $\alpha_c = 0$ for other states.

The results for energies and g -factors of xenon are presented in Table II. Note that the accuracy is similar to what we have for mercury. This is because the core-valence correlations are strong for mercury, they are significantly stronger than the correlations between two valence electrons. This is a limitation factor for the accuracy of the calculation. In contrast, the core-valence correlations are small for xenon.

A. Dalgarno-Lewis method for matrix elements

To calculate PNC amplitude we need to calculate matrix elements between many-electron states and perform summation over complete set of many-electron basis states (see, e.g. (6) and (7)). We use random phase approximation (RPA) [24, 25] for the matrix elements and Dalgarno-Lewis method [26] for the summation.

Matrix elements are given by

$$E1_{vw} = \langle \Psi_v | \hat{f} + \delta V_f | \Psi_w \rangle, \quad (12)$$

where δV is the correction to the core potential due to the core polarization by an external field \hat{f} . In present calculations \hat{f} represents either external electric field, SI weak interaction or SD PNC interaction.

Summation over complete set of many-electron states is reduced to calculation of the correction $\delta \Psi_v$ to the many-electron wave function of the state v due to the weak interaction perturbation H_{PNC} . Then, the PNC amplitude is given by

$$A_{vw} = \langle \delta \Psi_v | \mathbf{d} | \Psi_w \rangle. \quad (13)$$

The correction $\delta \Psi_v$ is found by solving the system of linear inhomogeneous equations

$$(\hat{H}^{\text{eff}} - E_v) \delta \Psi_v = -(\hat{H}_{\text{PNC}} + \delta V_{\text{PNC}}) \Psi_v. \quad (14)$$

The proposal of [12] considers the PNC transitions between the excited states A and B in Hg and Xe (see Tables I and II). The upper state B in both atoms is very close to another state of the same total momentum J but opposite parity. The interval is 8282 cm^{-1} for Hg and only 84 cm^{-1} in Xe. This is a strong advantage of using these transitions from the experimental point of view because the proximity of the states of the same total angular momentum but opposite parity leads to the strong enhancement of the PNC amplitude. On the other hand, this is a complication from the theoretical point of view. The PNC amplitudes are sensitive to small energy intervals where a small error in the calculated energy of the states can lead to a large error in the value of the PNC amplitude. To go around this problem we use a stabilizing procedure which consists of the following steps. First, we use the procedure described above (see Eq. (13) and (14)) without modifications. Then we repeat the calculations applying the orthogonality conditions for the $\delta \Psi_B$

to the close state of same J and parity. The contribution of the close state is found by comparing the two results. Finally, this contribution is added back to the PNC amplitude with the rescaling parameter $\Delta E_{\text{theor}}/\Delta E_{\text{exp}}$.

The procedure described above corresponds to the exact fitting of the energy denominators in (6) and (7). Therefore, the same results should be obtained if the important energy intervals are fitted exactly by rescaling the correlation potential $\hat{\Sigma}$ (for Hg) or polarization potential δV (for Xe). This is another important test which we used in the calculations.

B. Accuracy of the calculations

Accuracy of the similar calculations for two-valence-electron atoms Hg and Yb were discussed in detail in our earlier works [20, 21, 27]. It was demonstrated that the accuracy for transition amplitudes and polarizabilities is on the level of 5%. Note that the PNC amplitude is a second-order effect similar to polarizability but with one electric dipole operator replaced by weak interaction. In present work we assume the same 5% uncertainty for the PNC effect in mercury. This is supported by the study of the limitation factors which are discussed below.

The uncertainty for xenon is higher due to larger number of valence electrons which make it difficult to saturate the basis. We assume the 10% uncertainty which come from comparing the results obtained with two different basis sets, the b-spline basis set and the Hartree-Fock basis set.

The main factor limiting the accuracy of the calculations of the PNC amplitudes in xenon and mercury is the proximity of the levels of the same total momentum J and opposite parity. These states are mixed by weak interaction and small energy interval between them leads to strong enhancement of the PNC effect. This is one of the main reason for the choice of atoms and transitions. However, it represents a challenge for the calculations. Even small theoretical error in the energies of the mixed states can lead to large error in the PNC amplitude. There are two ways around this problem. One is to fit the energy interval exactly. Another is to isolate the resonant contribution from the rest of the amplitude and to re-scale it to the correct energy interval. We did both things for xenon and found that they give the same results. Therefore, for mercury we just fit the energies. As long as the problem of small energy intervals is understood and properly dealt with it didn't contribute much to the uncertainty of the results.

Another important limitation factor for xenon, which is harder to deal with, is large number of valence electrons. It was suggested in Ref. [12] that xenon can be treated as a system with one electron and one hole in the $5p$ subshell. This would make it a two-particle system similar to mercury. However, such approach assumes that only single excitations from the $5p$ subshell are considered. In our experience full saturation of the basis is

not possible without inclusion of double and may be even triple excitations. This would lead to the CI matrix of the extremely large size. Probably, this can be done with the use of supercomputers. Another open question for xenon is whether and how to include core-valence correlations. Incomplete saturation of the basis is the main source of the uncertainty of present calculations for xenon.

Saturation of the basis is not a problem for mercury when it is considered as a system with two valence electrons. However, here we have another problem, strong core-valence correlations. The outermost subshell of the mercury core, $5d$ is strongly mixed with the valence $6s$ electrons. This is evident from the presence in the discrete spectrum of mercury the states with excitations for the $5d$ subshell. The core-valence correlations are included in present work with the use of the second-order correlation operator $\hat{\Sigma}$. Most probably the correlations are too strong to be treated accurately within the second-order approach. The answer may come from the use of some all-order technique similar to what was recently developed in Ref. [28].

Even though some improvement of the accuracy of the calculations is possible, there is little chance that it will ever match the accuracy for cesium [5]. Therefore the main focus of the PNC study in Xe and Hg should be directed to the measurements of the anapole moments and to the study of the ratio of PNC effects in different isotopes.

IV. RESULTS AND DISCUSSION

The calculated nuclear spin-independent PNC amplitude for Xe (z -component) is

$$E_{\text{PNC}}(A \rightarrow B) = 1.76 \times 10^{-10}(-Q_W/N)iea_B. \quad (15)$$

The spin-independent PNC amplitudes for Hg are

$$\begin{aligned} E_{\text{PNC}}(A_1 \rightarrow B) &= 2.09 \times 10^{-10}(-Q_W/N)iea_B, \\ E_{\text{PNC}}(A_2 \rightarrow B) &= 1.77 \times 10^{-10}(-Q_W/N)iea_B, \\ E_{\text{PNC}}(A_3 \rightarrow B) &= 1.25 \times 10^{-10}(-Q_W/N)iea_B. \end{aligned} \quad (16)$$

The difference in the value of the PNC amplitude for different isotopes is mostly due to different value of the weak nuclear charge Q_W . Therefore, the amplitudes (15) and (16) may be used for any isotope.

Detailed data for both SD and SI PNC amplitudes for isotopes with non-zero nuclear spin are presented in Table III for Xe and Table IV for Hg.

A. M1 amplitudes

The experimental proposal [12] is aimed to measure the PNC optical rotation. The angle of rotation is proportional to the ratio $R = \text{Im}(E_{\text{PNC}}/M1)$. Therefore,

TABLE III: PNC amplitudes (z -components) for the $|5p^5 6s^2 \ ^2[3/2]_2^o, F_1\rangle \rightarrow |5p^5 6s^2 \ ^2[1/2]_1^o, F_2\rangle$ transitions in ^{129}Xe and ^{131}Xe . I is nuclear spin, $\mathbf{F} = \mathbf{J} + \mathbf{I}$. E' is given by (6).

A	I	E' units $10^{-10} iea_0$	F_1	F_2	PNC amplitude	
					$E'Q_W$	$10^{-10} iea_0$
129	1/2	3.16	3/2	1/2	$(1/3)(1 + 0.0387\kappa)$	$1.05(1 + 0.0387\kappa)$
			3/2	3/2	$-1/\sqrt{50}(1 + 0.010\kappa)$	$-0.45(1 + 0.010\kappa)$
			5/2	3/2	$\sqrt{2/25}(1 - 0.0226\kappa)$	$0.89(1 - 0.0226\kappa)$
131	3/2	3.25	1/2	1/2	$-1/\sqrt{18}(1 + 0.0345\kappa)$	$-0.766(1 + 0.0345\kappa)$
			1/2	3/2	$-1/\sqrt{90}(1 + 0.0252\kappa)$	$-0.343(1 + 0.0252\kappa)$
			3/2	1/2	$1/\sqrt{18}(1 + 0.0282\kappa)$	$0.766(1 + 0.0282\kappa)$
			3/2	3/2	$-\sqrt{8/125}(1 + 0.0189\kappa)$	$-0.822(1 + 0.0189\kappa)$
			3/2	5/2	$-1/\sqrt{375}(1 + 0.0034\kappa)$	$-0.178(1 + 0.0034\kappa)$
			5/2	3/2	$\sqrt{7/125}(1 + 0.0083\kappa)$	$0.769(1 + 0.0083\kappa)$
			5/2	5/2	$-\sqrt{3/70}(1 - 0.0072\kappa)$	$-0.673(1 - 0.0072\kappa)$
			7/2	5/2	$\sqrt{2/35}(1 - 0.0220\kappa)$	$0.777(1 - 0.0220\kappa)$

TABLE IV: PNC amplitudes (z -components) for the $|6s6p \ ^3P_J^o, F_1\rangle \rightarrow |6s6p \ ^1P_1^o, F_2\rangle$ transitions in ^{199}Hg and ^{201}Hg . I is nuclear spin, $\mathbf{F} = \mathbf{J} + \mathbf{I}$. E' is given by (6).

A	I	J	E' units $10^{-10} iea_0$	F_1	F_2	PNC amplitude	
						$E'Q_W$	$10^{-10} iea_0$
199	1/2	0	3.41	1/2	1/2	$(1/3)(1 + 0.0084\kappa)$	$1.14(1 + 0.0084\kappa)$
				1/2	3/2	$-\sqrt{2/9}(1 - 0.0042\kappa)$	$-1.61(1 - 0.0042\kappa)$
		1	5.31	1/2	1/2	$\sqrt{2/27}(1 + 0.0538\kappa)$	$1.44(1 + 0.0538\kappa)$
				1/2	3/2	$\sqrt{1/27}(1 - 0.0860\kappa)$	$1.02(1 - 0.0860\kappa)$
				3/2	1/2	$\sqrt{1/27}(1 + 0.0308\kappa)$	$1.02(1 + 0.0308\kappa)$
				3/2	3/2	$1/\sqrt{6}(1 - 0.0105\kappa)$	$2.17(1 - 0.0105\kappa)$
		2	3.71	3/2	1/2	$(1/3)(1 + 0.0381\kappa)$	$1.24(1 + 0.0381\kappa)$
				3/2	3/2	$-1/\sqrt{50}(1 + 0.0471\kappa)$	$-0.525(1 + 0.0471\kappa)$
				5/2	3/2	$\sqrt{2/25}(1 - 0.0264\kappa)$	$1.05(1 - 0.0264\kappa)$
				3/2	1/2	$(1/3)(1 + 0.0069\kappa)$	$1.16(1 + 0.0069\kappa)$
201	3/2	0	3.47	3/2	3/2	$1/\sqrt{5}(1 + 0.0028\kappa)$	$1.55(1 + 0.0028\kappa)$
				3/2	5/2	$-\sqrt{2/15}(1 - 0.0041\kappa)$	$-1.27(1 - 0.0041\kappa)$
				1/2	1/2	$-1/\sqrt{54}(1 + 0.0171\kappa)$	$-0.735(1 + 0.0171\kappa)$
				1/2	3/2	$\sqrt{5/54}(1 + 0.00362\kappa)$	$1.64(1 + 0.00362\kappa)$
				3/2	1/2	$\sqrt{5/54}(1 + 0.0419\kappa)$	$1.64(1 + 0.0419\kappa)$
				3/2	3/2	$\sqrt{2/75}(1 + 0.0607\kappa)$	$0.882(1 + 0.0607\kappa)$
		1	5.40	3/2	5/2	$(1/5)(1 - 0.0515\kappa)$	$1.08(1 - 0.0515\kappa)$
				5/2	3/2	$(1/5)(1 + 0.0122\kappa)$	$1.08(1 + 0.0122\kappa)$
				5/2	5/2	$1/\sqrt{6}(1 - 0.0103\kappa)$	$2.20(1 - 0.0103\kappa)$
		2	3.78	1/2	1/2	$-1/\sqrt{18}(1 + 0.0385\kappa)$	$-0.890(1 + 0.0385\kappa)$
				1/2	3/2	$-1/\sqrt{90}(1 + 0.0414\kappa)$	$-0.398(1 + 0.0414\kappa)$
				3/2	1/2	$1/\sqrt{18}(1 + 0.0240\kappa)$	$0.890(1 + 0.0240\kappa)$
				3/2	3/2	$-\sqrt{8/125}(1 + 0.0269\kappa)$	$-0.956(1 + 0.0269\kappa)$
				3/2	5/2	$-1/\sqrt{375}(1 + 0.0318\kappa)$	$-0.195(1 + 0.0318\kappa)$
				5/2	3/2	$\sqrt{7/125}(1 + 0.00286\kappa)$	$0.894(1 + 0.00286\kappa)$
				5/2	5/2	$-\sqrt{3/70}(1 + 0.00774\kappa)$	$-0.782(1 + 0.00774\kappa)$
				7/2	5/2	$\sqrt{2/35}(1 - 0.0260\kappa)$	$0.903(1 - 0.0260\kappa)$

we need to know the values of the magnetic dipole amplitudes for the transitions proposed for PNC measurements. The most accurate values of the M1 amplitudes can be found analytically using experimental values of the magnetic g -factors to find the coefficients for configuration mixing.

This is especially important for the case of mercury where numerical calculations of the M1 amplitudes give unstable results. The reason for this instability is easy to understand. The transitions considered for the PNC measurements in mercury are between states of different spin ($S = 1$ for states $A_{1,2,3}$ and $S = 0$ for state B).

This means that the M1 amplitudes between these states vanish in the non-relativistic limit. In relativistic calculations the amplitudes are not zero but small. These small values are obtained as a result of strong cancelation between different contributions. This strong cancelation leads to unstable results.

On the other hand analytical evaluation of the M1 amplitudes is simple and produce very accurate results. The operator of the magnetic dipole transition ($M_z = (L_z + 2S_z)\mu_B$) has no radial part and cannot change a principal quantum number in the non-relativistic limit. Therefore, the magnetic g -factors and M1 amplitudes are mainly sensitive to the mixing of the states belonging to the same configuration. Mixing with other configurations normally produces corrections at the 10^{-3} level [29]. We may see this in Table I and II where g -factors of "pure" sp states with $J = 2$ and sum of the g -factors for mixed states $J = 1$ differ from the experimental values by less than 0.1 %. Therefore, the mixing coefficients for the states belonging to the same configuration and M1 amplitudes can be found practically exactly from the known values of the g -factors. Note that we use the calculated value of the overlap between the radial wave functions $p_{1/2}$ and $p_{3/2}$ which is close but not equal to 1. For Hg it is 0.988.

We get for the states A and B of xenon

$$\begin{aligned}\Psi_A &= |5p_{3/2}6s\rangle \\ \Psi_B &= 0.05|5p_{3/2}6s\rangle + 0.999|5p_{1/2}6s\rangle.\end{aligned}\quad (17)$$

This leads to the M1 amplitude

$$M1_{AB} = 1.22\mu_B = 0.00446ea_B. \quad (18)$$

Using E' from table III we get $R = 7.1(7)(35) \times 10^{-8}$ for ^{129}Xe and $R = 7.3(7) \times 10^{-8}$ for ^{131}Xe . Here we assume the 10% uncertainty as it has been discussed above. These values of $M1$ and R are close but not in perfect agreement to what was found in Ref. [12]: $M1 = 0.0042ea_B$, $R = 11(3) \times 10^{-8}$. The reason for difference in $M1$ is not clear. The authors of Ref. [12] use slightly different coefficients of configuration mixing in (17). Their values are 0.062 and 0.998. However, if we use these coefficients we get $M1 = 0.00444ea_B$ which is different from the value $M1 = 0.0042ea_B$ presented in Ref. [12].

The situation is more complicated for mercury. All the M1 transitions of interest happen between the states with different total spin and vanish in the non-relativistic limit since the operator $L_z + 2S_z$ conserves the total spin. This leads to the strong suppression. The values of the M1 amplitudes presented in Ref. [12] are too large for the spin-forbidden transitions. No choice of the configuration mixing coefficients can reproduce them.

The wave functions for states $A_{1,2,3}$ and B for Hg have

the form

$$\begin{aligned}\Psi_{A_1} &= |6p_{1/2}6s\rangle \\ \Psi_{A_2} &= 0.432|6p_{3/2}6s\rangle - 0.902|6p_{1/2}6s\rangle, \\ \Psi_{A_3} &= |6p_{3/2}6s\rangle. \\ \Psi_B &= 0.902|6p_{3/2}6s\rangle + 0.432|6p_{1/2}6s\rangle,\end{aligned}\quad (19)$$

The coefficients 0.902 and 0.432 are chosen to fit the experimental g -factors of the states A_2 and B. When projections are included all $|^{2S+1}P_{J_z}\rangle$ states of the $6s6p$ configuration can be written as

$$\begin{aligned}|A_1 : ^3P_{00}^o\rangle &= -\frac{1}{\sqrt{2}} \left[|6s_{\frac{1}{2}\frac{1}{2}}6p_{\frac{1}{2}-\frac{1}{2}}\rangle - |6s_{\frac{1}{2}-\frac{1}{2}}6p_{\frac{1}{2}\frac{1}{2}}\rangle \right], \\ |A_2 : ^3P_{11}^o\rangle &= -0.216|6s_{\frac{1}{2}\frac{1}{2}}6p_{\frac{3}{2}\frac{1}{2}}\rangle + \\ &\quad 0.374|6s_{\frac{1}{2}-\frac{1}{2}}6p_{\frac{3}{2}\frac{3}{2}}\rangle + 0.902|6s_{\frac{1}{2}\frac{1}{2}}6p_{\frac{1}{2}\frac{1}{2}}\rangle, \\ |A_3 : ^3P_{22}^o\rangle &= |6s_{\frac{1}{2}\frac{1}{2}}6p_{\frac{3}{2}\frac{3}{2}}\rangle, \\ |B : ^1P_{11}^o\rangle &= -0.451|6s_{\frac{1}{2}\frac{1}{2}}6p_{\frac{3}{2}\frac{1}{2}}\rangle + \\ &\quad 0.781|6s_{\frac{1}{2}-\frac{1}{2}}6p_{\frac{3}{2}\frac{3}{2}}\rangle - 0.432|6s_{\frac{1}{2}\frac{1}{2}}6p_{\frac{1}{2}\frac{1}{2}}\rangle.\end{aligned}\quad (20)$$

Here we use (19) for the expansion. The results for M1 amplitudes obtained with the use of these formulas are presented in Table V together with the values from Ref. [12]. Note that there must be $M1 \ll \mu_B$ for the spin-forbidden transitions. This holds for the results of present work but not for the results of Ref. [12]. Table V also presents the PNC amplitudes and the ratios $R = \text{Im}(E_{\text{PNC}}/M1)$. The numbers include 5% error bars according to the estimated uncertainty of the calculations which was discussed in section III B. Note that the values of the M1 amplitudes obtained in the present work are practically exact due to the fitting of the experimental g -factors.

The values of the ratios R are larger than in Ref. [12] due to smaller M1 amplitudes. The values of R for mercury are about an order on magnitude larger than for xenon (see above) and about an order of magnitude larger than for Tl, Pb and Bi [30–32].

B. Optical rotation

The angle of optical rotation is given by [33]

$$\phi_{\text{PNC}} = -\frac{4\pi l}{\lambda} (n(\omega) - 1) R, \quad (21)$$

where l is path length in vapor, λ is wavelength of laser light, ω is its frequency, and $n(\omega)$ is refractive index due to the absorption. Although the angle is proportional to the ratio $R = \text{Im}(E_{\text{PNC}}/M1)$, the small values for the M1 amplitudes do not necessarily translate into a large angle of rotation. This is because the refractive index also depends on $M1$ amplitude, $n(\omega) - 1 \sim |M1|^2$, which leads to $\phi \sim M1 \cdot E_{\text{PNC}}$. However, the suppression due to the small M1 amplitude can be compensated at

TABLE V: Magnitudes of the M1 and PNC amplitudes (reduced matrix elements) and ratios $R \equiv Im(E_{PNC}/M1)$ for the $^3P_J - ^1P_1$ transitions in mercury. Values for M1 from Ref. [12] are also presented for comparison.

Transition	M1 amplitudes				$Im(E_{PNC})$		R	
	This work		Ref. [12]		^{199}Hg	^{201}Hg	^{199}Hg	^{201}Hg
	units $10^{-4}ea_B$	μ_B	$10^{-4}ea_B$	μ_B	$10^{-10}ea_B$	$10^{-10}ea_B$	10^{-7}	10^{-7}
$^3P_0^o - ^1P_1^o$	8.37	0.229	14	0.384	3.4(2)	3.5(2)	4.1(2)	4.2(2)
$^3P_1^o - ^1P_1^o$	7.26	0.199	42	1.15	5.3(3)	5.4(3)	7.3(4)	7.4(4)
$^3P_2^o - ^1P_1^o$	9.94	0.272	57	1.56	3.7(2)	3.8(2)	3.7(2)	3.8(2)

sufficiently high vapor pressure by the appropriate choice of the path length l . These questions are discussed in detail in Ref. [33]. Here we just note that the angle of rotation per unit length is $\phi \sim M1 \cdot E_{PNC}$. However, the angle of rotation per absorption length $\phi \sim R$ and it is large for small M1.

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